feeling. Cocoa butter consists mainly of three triacylglycerols (TAGs): 1,3-dipalmitoyl-2-oleoylglycerol (POP), 1-palmitoyl-2-oleoyl-3-stearoylglycerol (POS) and 1,3-di-stearoyl-2-oleoylglycerol (SOS). Besides, smaller amounts of mono-, di-glycerides and free fatty acids are present.
The TAG composition of cocoa butter or a fat in general is one of the most important parameters since it governs the physical properties and determines its polymorphic form. Polymorphism is defined here as the ability of the TAG molecules to crystallize in different molecular packing arrangements corresponding to different unit cell structures. Fat polymorphs are typically classified by three main forms (α, β', β and variations within these types). The different polymorphs determine the physical-chemical properties and hence the texture, long-term stability and consequently shelf-life of the products used in technological applications. In a combined synchrotron small- and wide-angle x-ray scattering (SAXS/WAXS) study, we have explored the use of the thermodynamic parameter pressure in modulating and controlling these properties, and to determine the temperature-pressure phase diagram of a triglyceride system.

1942-Pos Board B672
Unraveling the Heparin-Induced Protofibril Structure of GAPDH
Rosangela Itri[1], Elisa M. Sales[1], Leandro R.S. Barbosa[1], Clarisa M. Torres-Bugeau[2], César L. Ávila[2], Rosana N. Chehín[2].
[1]Física Aplicada, Instituto de Física, São Paulo, Brazil, [2]Instituto Superior de Investigaciones Biológicas (INSIBIO), Tucuman, Argentina.
Citotoxicity in Parkinson disease has been linked to an oligomeric arrangement of the protein α-synuclein (α-SN), which can alter the membrane permeability. In this work we could demonstrate the ability of heparin-induced Gliceraldehyde-3-phosphate dehydrogenase (GAPDH) aggregates to modulate the effect of oligomeric α-SN species on cell survival and membrane stability. From the GAPDH species formed after heparin addition, a cylinder-shaped protofibril species with an average length of 22 nm and a diameter of 12 nm are able to sequester α-SN oligomers. Using biocomputational techniques we obtained the first all-atom model of the GAPDH protofibril capable to satisfy experimental restrictions deduced from small angle X-ray scattering and mass spectrometry. We also propose a fibrillation pathway for the heparin-induced GAPDH aggregation. Upon heparin binding to GAPDH, the tetrameric state of the enzyme is lost and native-like dimer species appeared. The formed dimers are the building block of higher orders aggregates, which in a very fast way assemble to hexamers that piling up allowing the formation of the protofibrilar species.

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Optical Scattering of Liposomes Suspended above a Surface
Pieter A.A. De Beule.
Applied Nano-Optics Laboratory, International Iberian Nanotechnology Laboratory, Braga, Portugal.
Lipid bilayers exhibit a different refractive index parallel and perpendicular to their surface. This optical birefringence is characteristic for the size, shape and orientation of the lipid molecules in the membrane [1].
A new optical model to investigate the optical birefringence of liposomes suspended above a surface is presented. The solution to Maxwell's equation for particles suspended above a surface, as presented by Bobbert and Vlieger [2], is extended to investigate the optical scattering properties of liposomes suspended above a surface. Numerical simulations demonstrate that ellipsometry is highly sensitive to the distance of liposomes above a surface and that ellipsometry can be applied to determine the optical anisotropy of the liposome lipid bilayer, creating opportunities for the use of ellipsometry in the investigation of the supported lipid bilayer formation process.
The optical model also allows for the analysis of more complex structures such as nanoparticles coated with a lipid bilayer, or liposomes whose lumen contains a spherical nanoparticle. The influence of the presence of a lipid bilayer and its optical anisotropy on ellipsometry measurements is presented. Also, it is investigated how model parameters such as lipid bilayer anisotropy can be experimentally separated from other model parameters such as e.g. the overall particle radius.
[1] Z. Salamon and G. Tollin, Biophysical Journal, 80, 1557-1569 (2001); [2] P. Bobbert and J. Vlieger, Physica A: Statistical Mechanics and its Applications, 137A, 209-242 (1986)

1944-Pos Board B674
The Effect of Magnesium on the Thermodynamics of Nucleic Acid Tertiary Contact Formation
Herschel M. Watkins, Derek Mendez, Daniel Ratner, Daniel Herschlag, Sebastian Doniach.
Stanford University, Stanford, CA, USA.
Functional RNAs fold into compact, well-defined tertiary structures despite strong electrostatic repulsion both within and between helices. To achieve these compact structures, many RNAs employ structural divalent cations, typically Mg^{2+}. The simplest tertiary contact in nucleic acids is two helices, joined by some non-helical contact. To explore the fundamental characteristics of tertiary contact formation in nucleic acids we studied a system of two DNA helices tethered via a short PEG linker by both computational and experimental methods. Computationally, we predict the electrostatic repulsion between these helices as a function of Mg^{2+} and Na^{+} concentration. Experimentally, we linked the distal termini of these helices via a disulfide linker. Using small-angle x-ray scattering, we measured the fraction of intact disulfide bonds as a function of reducing strength of the buffer at a range of Mg^{2+} and Na^{+} concentration. Using these data we can extrapolate the magnitude of the strain on the disulfide bond, and thus the repulsion between the helices. Previous results show that the conformational ensemble is narrowly distributed around an extended, co-linear conformation at low salt and becomes more relaxed at high salt, but is unable to isolate a conformation in which the helices are stacked. Furthermore, previous results also suggest that specific interactions between Mg^{2+} and the phosphate backbone strongly are more important than simple ionic strength in determining the magnitude of the repulsive potential between the helices. In this project, we hope to experimentally demonstrate the energy of helix stacking and the different role of ionic strength and ionic specific interactions.

1945-Pos Board B675
Asymmetric Illumination of Optically Anisotropic Beads for Detecting Rotational Motion
Chang Jiang, Edgar Meyhofer.
University of Michigan, Ann Arbor, MI, USA.
Many biological molecules, including RNA polymerases and ATP synthases, undergo rotational motion during their biological processes. Characterizing these processes at the single molecule level with high temporal and spatial resolution can reveal valuable information about their mechanical and dynamical properties. We are particularly interested in the dynamics of conformational changes of DNA molecules under torsion. Toward this long term goal we have developed a methodology that enables us to directly record the angular displacement of particles undergoing rotational motion by using asymmetric illumination of optically anisotropic beads. The method is implemented by illuminating a partially metal-coated bead with a laser beam coupled into the back side of the objective. The laser beam illuminating beads in the sample plane is oriented at an oblique angle to form asymmetric illumination. We observe that the scattering signal of the bead changes with the angular displacement of the coating on the bead relative to the illuminating laser beam. We use an optoelectronic system to detect scattering signal which is the direct high-speed measurement of the angular displacement of the bead. We conclude that our method is able to map angular displacements to electrical signal and we can determine the angular displacement of the biological molecule when conjugated to the bead. Our method obviates image acquisition and image processing procedures commonly used in previous studies, and it has the potential to significantly enhance the bandwidth of detection. We envision usage of this method in a range of biophysical measurements including magnetic trapping, tethered particle motion. We plan to use this rotational tracking method in combination with magnetic tweezers, a single-molecule technique that enables the application of torsional stress to twist single DNA molecules to extract high bandwidth torsional mechanical properties and dynamics of the molecules.

Force Spectroscopy

1946-Pos Board B676
Investigating Protein-Protein Interaction Networks with Force Spectroscopy
Oliver E. Farrance[1], Renata Kaminska[2], Nicholas G. Housden[2], Sasha R. Derrington[1], Colin Kleanthous[2], Sheena E. Radford[1], David J. Brockwell[1].
[1]University of Leeds, Leeds, United Kingdom, [2]University of Oxford, Oxford, United Kingdom.
Colicins are antimicrobial proteins produced by bacteria. Their highly active modes of killing make colicins of interest as a potential new class of antibiotics. However, the precise mechanism of cytotoxicity is not understood thus limiting their translation to biotechnological applications.
It is thought that colicin intoxication occurs via a series of protein-protein interactions (PPIs) that span the periplasm (Housden et al. Science, 2013). Mechanical force may play a role in this process by an inside-out energy transduction mechanism. Periplasmic proteins that are subverted by colicins have either a known role in applying force during their normal function *in-vivo* or are highly homologous to proteins that do.